

# Short distance correlators in the XXZ spin chain for arbitrary string distributions

Márton Mestyán<sup>1</sup>, Balázs Pozsgay<sup>1</sup>

<sup>1</sup>MTA–BME "Momentum" Statistical Field Theory Research Group  
1111 Budapest, Budafoki út 8, Hungary

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## Abstract

In this letter we consider expectation values of local correlators in highly excited states of the spin-1/2 XXZ chain. Assuming that the string hypothesis holds we formulate the following conjecture: The correlation functions can be computed using the known factorized formulas of the finite temperature situation, if the building blocks are computed via certain linear integral equations using the string densities only. We prove this statement for the nearest neighbour z-z correlator for states with arbitrary string densities. Also, we check the conjecture numerically for other correlators in the finite temperature case. Our results pave the way towards the computation of the stationary values of correlators in non-equilibrium situations using the quench action approach.

## 1 Introduction

The analytical calculation of correlation functions of the spin-1/2 XXZ chain is by now a very advanced subject. There are multiple integral formulas available for mean values of local operators for both the ground state [1, 2] and in the finite temperature case [3]. Moreover it is known that these multiple integrals can be factorized, i.e. they can be expressed as sums of products of simple integrals (see [4] and references therein). This provides a very efficient way for the numerical evaluation of the local correlations.

Previous research on this subject only considered the ground state or finite temperature mean values. However, recent advances in the study of non-equilibrium processes provide motivation to determine the correlations in more general situations, for example in the case of quantum quenches [5]. Ideally one would like to obtain exact results for the time-dependent correlators after a quench, but this is beyond the reach of the present methods. A simpler task is derive the mean values in the long-time limit.

The Generalized Gibbs Ensemble (GGE) hypothesis [6] states that the stationary values of local correlators can be evaluated using a modified statistical ensemble which incorporates all higher local charges of the model with appropriate Lagrange multipliers. The papers [7, 8, 9] developed generalizations of the Quantum Transfer Matrix method (originally devised for the finite temperature problem [10]) to compute local correlators in the GGE for quantum quenches in the XXZ chain. While [7] and [8] employed approximations, the authors of [9] were able to calculate the exact predictions of the GGE in a number of different cases. It is important to note that all of these papers used the factorized formulas for the correlators found in [11].

In [5] a different approach was suggested which is based on first principles. If the overlaps between the initial state and the eigenstates of the final Hamiltonian are known, then the analysis of the so-called quench action (overlaps and entropy combined) provides the Bethe root distributions of sample states which determine the time evolution at large times. Such a calculation is completely analogous to the minimalization of the free energy using the Thermodynamic Bethe Ansatz (TBA), but the resulting root distributions are typically very different from the thermal case [12].

Concerning the XXZ chain one drawback of the quench action approach is that it only provides the string densities, but up to now it has not been known how to compute the correlation functions which are the actual measurable quantities. Here we make an attempt to fill this gap. Our work is partly motivated by the papers [13, 14] where simple determinant formulas have been found for the overlaps between the Néel state and the Bethe states, thus making the determination of the saddle point distributions possible [15, 16, 17].

The paper is organized as follows. In Section 2 we introduce the model and its coordinate Bethe Ansatz solution. In Section 3 we compute an integral formula for the nearest neighbour z-z correlator, which holds for an arbitrary distribution of Bethe roots. The finite temperature situation is considered in Section 4, where we present the QTM formulas for the local correlators and the TBA result for  $\langle \sigma_1^z \sigma_2^z \rangle_T$ . In Section 5 we introduce a generalization of the formulas of Section 2 and present two Conjectures for the local correlators. Finally, Section 6 includes the discussion of our results. Numerical data for the correlators in the finite temperature case are presented in the Appendix.

## 2 Eigenstates and root densities

Consider the XXZ spin-1/2 chain with Hamiltonian

$$H_{XXZ} = \sum_{j=1}^L \left\{ \sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta (\sigma_j^z \sigma_{j+1}^z - 1) \right\} + h \sum_{j=1}^L (\sigma_j^z - 1). \quad (2.1)$$

Here  $h$  is a longitudinal magnetic field and  $\Delta = \cosh(\eta)$  is the anisotropy parameter. For simplicity we only consider the regime with  $\Delta > 1$  where  $\eta \in \mathbb{R}^+$ . In this work periodic boundary conditions are assumed.

Eigenstates can be constructed by the different forms of the Bethe Ansatz [18]. Choosing the vector  $|F\rangle = |++\cdots+\rangle$  as a reference state an eigenstate with  $N$  down spins can be characterised by a set of rapidities (quasi-momenta)  $\{\lambda_1, \dots, \lambda_N\}$  which describe the propagation of the interacting spin waves. In coordinate Bethe Ansatz the explicit wave function can be written as

$$\Psi_N(\lambda_1, \dots, \lambda_N | s_1, \dots, s_N) = \sum_{P \in \sigma_N} \prod_j \left( \frac{\sin(\lambda_{P_j} + i\eta/2)}{\sin(\lambda_{P_j} - i\eta/2)} \right)^{s_j} \prod_{j>k} \frac{\sin(\lambda_{P_j} - \lambda_{P_k} - i\eta)}{\sin(\lambda_{P_j} - \lambda_{P_k})}. \quad (2.2)$$

Here  $s_j$  denote the positions of the down spins, and we assume  $s_j < s_k$  for  $j < k$ . Periodic boundary conditions impose the Bethe equations:

$$P(\lambda_j)^L \prod_{k \neq j} S(\lambda_j - \lambda_k) = 1, \quad (2.3)$$

where

$$P(\lambda) = e^{ip(\lambda)} = \frac{\sin(\lambda + i\eta/2)}{\sin(\lambda - i\eta/2)}$$

is the propagator of a single down spin and the function

$$S(\lambda) = \frac{\sin(\lambda - i\eta)}{\sin(\lambda + i\eta)}$$

describes the scattering of the spin waves.

If the Bethe equations hold then the energy eigenvalue is given by

$$E_\Psi = -2Nh + \sum_j e(\lambda_j), \quad \text{where} \quad e(u) = \frac{4 \sinh^2 \eta}{\cos(2u) - \cosh \eta}. \quad (2.4)$$

The string hypothesis [19] states that in a large volume typical eigenstates consists of spin waves with real rapidities  $\lambda_j$  and/or bound states of  $n$  spin waves such that the rapidities of the constituents are

$$\{\lambda\}_n = x - \frac{n-1}{2}i\eta + i\delta_1, x - \frac{n-3}{2}i\eta + i\delta_2, \dots, x + \frac{n-1}{2}i\eta + i\delta_n.$$

Here  $x \in [-\pi/2, \pi/2]$  is called the string center and the parameters  $\delta_j$  are string deviations which are exponentially small in  $L$  and can be neglected in the thermodynamic limit.

The string hypothesis allows us to write down a set of equations for the string centers only. Let us assume that the Bethe state consists of  $n$  "particles" such that the string lengths are  $\alpha_k$ ,  $k = 1 \dots n$ , and the string centers are given by  $x_k$ . The total number of down spins is

$$N = \sum_{k=1}^n \alpha_k.$$

Then we have

$$P_{\alpha_j}(x_j)^L \prod_{k \neq j} S_{\alpha_j \alpha_k}(x_j - x_k) = 1, \quad j = 1 \dots n. \quad (2.5)$$

Here

$$P_\alpha(\lambda) = \frac{\sin(\lambda + i\alpha\eta/2)}{\sin(\lambda - i\alpha\eta/2)}$$

and

$$S_{nm} = \begin{cases} P_{-|n-m|}(P_{-(|n-m|+2)}P_{-(|n-m|+4)} \dots P_{-(n+m-2)})^2 P_{-(n+m)} & \text{if } m \neq n \\ (P_{-2}P_{-4} \dots P_{-(2n-2)})^2 P_{-2n} & \text{if } m = n. \end{cases}$$

The set (2.5) is called the Bethe-Takahashi equations.

Consider a large volume  $L$  with a large number of particles such that  $N/L = \mathcal{O}(1)$ . In typical eigenstates the string centers are distributed smoothly for each type of string. Let us introduce the density of roots of  $j$ -strings  $\rho_{r,j}^{(0)}$  and total density of  $j$ -string roots and holes  $\rho_j^{(0)}$ . The superscript (0) is introduced for later convenience. These functions satisfy the constraint following from the Bethe-Takahashi equations:

$$\rho_k^{(0)}(u) = -s_k^{(0)}(u) - \sum_{l=1}^{\infty} \int_{-\pi/2}^{\pi/2} \frac{d\omega}{2\pi} \varphi_{kl}(u - \omega) \rho_{r,l}^{(0)}(\omega). \quad (2.6)$$

Here

$$s_k^{(0)}(u) = (-i) \frac{\partial}{\partial u} \log P_k(u) = (-i) [\cot(u + ik\eta/2) - \cot(u - ik\eta/2)]$$

and  $\varphi_{nm}(u) = \frac{\partial}{\partial u} (-i) \log S_{nm}(u)$ . Explicitly

$$\varphi_{nm} = \begin{cases} -(s_{|n-m|}^{(0)} + 2s_{|n-m|+2}^{(0)} + 2s_{|n-m|+4}^{(0)} + \dots + 2s_{n+m-2}^{(0)} + s_{n+m}^{(0)}) & \text{if } m \neq n \\ -(2s_2^{(0)} + 2s_4^{(0)} + \dots + 2s_{2n-2}^{(0)} + s_{2n}^{(0)}) & \text{if } m = n. \end{cases} \quad (2.7)$$

The total number of down spins is given by

$$\frac{N}{L} = \sum_{k=1}^{\infty} k \int \frac{du}{2\pi} \rho_{r,k}^{(0)}(u).$$

It is useful to define the functions  $\eta_k(u)$  as

$$\frac{1}{1 + \eta_k(u)} = \frac{\rho_{r,k}^{(0)}(u)}{\rho_k^{(0)}(u)} \quad (2.8)$$

such that (2.6) can be written as

$$\rho_k^{(0)}(u) = -s_k^{(0)}(u) - \sum_{l=1}^{\infty} \int_{-\pi/2}^{\pi/2} \frac{d\omega}{2\pi} \varphi_{kl}(u - \omega) \frac{\rho_l^{(0)}(\omega)}{1 + \eta_l(\omega)}. \quad (2.9)$$

The ratio  $1/(1 + \eta_k)$  can be interpreted as a "filling fraction" for the  $k$ -string centers.

We note that the functions  $s_k^{(0)}$  are proportional to the  $j$ -string energies which follows from the fact that for a single rapidity

$$e(\lambda) = 2 \sinh(\eta) s_1^{(0)}(\lambda).$$

For further use we introduce the operator

$$Q_2 = \frac{1}{2 \sinh \eta} H \quad (2.10)$$

whose single-particle eigenfunctions coincide with  $s_j^{(0)}$ :

$$\langle Q_2 \rangle_{\Psi} = \sum_{j=1}^N s_1^{(0)}(\lambda_j) = \sum_{k=1}^n s_{\alpha_k}^{(0)}(x_k).$$

In a large volume this relation can be written as

$$\frac{\langle Q_2 \rangle_{\Psi}}{L} = \sum_{k=1}^{\infty} \int \frac{du}{2\pi} s_k^{(0)}(u) \rho_{r,k}^{(0)}(u).$$

To conclude this section we introduce a simplified notation for the various convolutions and integrals which appear in this work. Linear integral equations of the type

$$f_k(u) = g_k(u) - \sum_{l=1}^{\infty} \int_{-\pi/2}^{\pi/2} \frac{d\omega}{2\pi} \varphi_{kl}(u - \omega) \frac{f_k(\omega)}{1 + \eta_k(\omega)} \quad (2.11)$$

will be denoted by

$$f = g - \varphi \star \frac{f}{1 + \eta}. \quad (2.12)$$

Also, integrals of the type

$$I = \sum_{k=1}^{\infty} \int \frac{du}{2\pi} f_k(u) \frac{g_k(u)}{1 + \eta_k(u)}$$

will be denoted by

$$I = f \cdot \frac{g}{1 + \eta}.$$

With these notations the equations for the string densities read

$$\rho^{(0)} = -s^{(0)} - \varphi \star \frac{\rho^{(0)}}{1 + \eta}, \quad (2.13)$$

whereas the expectation value of  $Q_2$  is expressed as

$$\frac{\langle Q_2 \rangle_{\Psi}}{L} = s^{(0)} \cdot \frac{\rho^{(0)}}{1 + \eta}.$$

### 3 $\langle \sigma_1^z \sigma_2^z \rangle_\Psi$ from the Hellmann–Feynman theorem

In this section we obtain an integral formula for the mean value  $\langle \sigma_1^z \sigma_2^z \rangle_\Psi$  for arbitrary excited states with a smooth density of roots.

Consider an eigenstate

$$|\Psi\rangle = |\{\lambda\}_N\rangle$$

in a finite spin chain of length  $L$ . We apply the Hellmann–Feynman theorem [20] for this particular state, such that we choose  $\Delta$  as the variation parameter:

$$\langle \Psi | \partial H / \partial \Delta | \Psi \rangle = L \langle \Psi | (\sigma_1^z \sigma_2^z - 1) | \Psi \rangle = \frac{\partial E_\Psi}{\partial \Delta}.$$

It is convenient to express the energy in terms of the  $Q_2$  eigenvalue as given by the relation (2.10). Using  $\Delta = \cosh(\eta)$  we obtain

$$L \langle \Psi | (\sigma_1^z \sigma_2^z - 1) | \Psi \rangle = 2 \coth(\eta) \langle Q_2 \rangle_\Psi + 2 \frac{\partial \langle Q_2 \rangle_\Psi}{\partial \eta}.$$

In the following we evaluate the derivative on the r.h.s. in the finite volume case and take the thermodynamic limit afterwards.

#### 3.1 States consisting of one-strings only

First we consider the cases when the state  $|\Psi\rangle$  consists of 1-strings only. Taking the derivative of the logarithm of the Bethe equations (2.3) with respect to  $\eta$  leads to

$$0 = L \tilde{s}^{(0)}(\lambda_j) + L f(\lambda_j) s^{(0)}(\lambda_j) + \sum_{k \neq j} \tilde{\varphi}(\lambda_j - \lambda_k) + \sum_{k \neq j} (f(\lambda_j) - f(\lambda_k)) \varphi(\lambda_j - \lambda_k), \quad (3.1)$$

where we introduced the "shift function"  $f(\lambda)$  by

$$\frac{\partial \lambda_j}{\partial \eta} = f(\lambda_j)$$

and

$$\begin{aligned} \tilde{s}^{(0)}(u) &= (-i) \frac{\partial}{\partial \eta} \log P(u) = \\ &= \frac{1}{2} [\cot(u + i\eta/2) + \cot(u - i\eta/2)] = \frac{\sin(2u)}{2 \sin(u - i\eta/2) \sin(u + i\eta/2)} \\ \tilde{\varphi}(u) &= (-i) \frac{\partial}{\partial \eta} \log S(u) = \\ &= -[\cot(u + i\eta) + \cot(u - i\eta)] = \frac{-\sin(2u)}{\sin(u - i\eta) \sin(u + i\eta)}. \end{aligned} \quad (3.2)$$

In the thermodynamic limit (3.1) is written as

$$0 = \tilde{s}^{(0)}(\lambda) + f(\lambda) s^{(0)}(\lambda) + \int \frac{d\omega}{2\pi} \rho_r^{(0)}(\omega) \tilde{\varphi}(\lambda - \omega) + \int \frac{d\omega}{2\pi} \rho_r^{(0)}(\omega) (f(\lambda) - f(\omega)) \varphi(\lambda - \omega). \quad (3.3)$$

In the 1-string case the densities satisfy

$$\rho^{(0)}(u) = -s^{(0)}(u) - \int \frac{d\omega}{2\pi} \varphi(u - \omega) \rho_r^{(0)}(\omega) \quad (3.4)$$

with  $\varphi(u) = \varphi_{11}(u)$ . Substituting (3.4) to (3.3) leads to

$$0 = \tilde{s}^{(0)}(\lambda) - f(\lambda)\rho^{(0)}(\lambda) + \int \frac{d\omega}{2\pi} \rho_r^{(0)}(\omega) \tilde{\varphi}(\lambda - \omega) - \int \frac{d\omega}{2\pi} \rho_r^{(0)}(\omega) f(\omega) \varphi(\lambda - \omega). \quad (3.5)$$

This equation uniquely determines  $f(\lambda)$ . The variation of  $Q_2$  is then expressed as

$$\frac{\partial \langle Q_2 \rangle_\Psi}{\partial \eta} = \sum \tilde{s}^{(1)}(\lambda_j) + \sum s^{(1)}(\lambda_j) f(\lambda_j), \quad (3.6)$$

where

$$\begin{aligned} \tilde{s}^{(1)}(u) &= \frac{\partial s^{(0)}(u)}{\partial \eta} = -\frac{1}{2} \left[ \frac{1}{\sin^2(u + i\eta/2)} + \frac{1}{\sin^2(u - i\eta/2)} \right] \\ s^{(1)}(u) &= \frac{\partial s^{(0)}(u)}{\partial u} = i \left[ \frac{1}{\sin^2(u + i\eta/2)} - \frac{1}{\sin^2(u - i\eta/2)} \right]. \end{aligned}$$

In the thermodynamic limit (3.6) is expressed as

$$\frac{1}{L} \frac{\partial \langle Q_2 \rangle_\Psi}{\partial \eta} = \int \frac{du}{2\pi} (\tilde{s}^{(1)}(u) \rho_r^{(0)}(u) + s^{(1)}(u) f(u) \rho_r^{(0)}(u)). \quad (3.7)$$

Introducing the function

$$\sigma^{(0)}(u) = f(u) \rho^{(0)}(u)$$

and using the definition (2.8) for the 1-strings we have

$$0 = \tilde{s}^{(0)}(\lambda) - \sigma^{(0)}(\lambda) + \int \frac{d\omega}{2\pi} \rho_r^{(0)}(\omega) \tilde{\varphi}(\lambda - \omega) - \int \frac{d\omega}{2\pi} \frac{\sigma^{(0)}(\omega)}{1 + \eta(\omega)} \varphi(\lambda - \omega) \quad (3.8)$$

and

$$\frac{1}{L} \frac{\partial \langle Q_2 \rangle_\Psi}{\partial \eta} = \int \frac{du}{2\pi} \left( \tilde{s}^{(1)}(u) \frac{\rho^{(0)}(u)}{1 + \eta(u)} + s^{(1)}(u) \frac{\sigma^{(0)}(u)}{1 + \eta(u)} \right). \quad (3.9)$$

The expectation value of  $Q_2$  is simply

$$\frac{\langle Q_2 \rangle_\Psi}{L} = \int \frac{du}{2\pi} s^{(0)}(u) \rho_r^{(0)}(u).$$

Putting everything together the final result for the mean value can be written as

$$\langle \sigma_1^z \sigma_2^z \rangle_\Psi = 1 - \coth(\eta) \Omega_{0,0} + \Gamma_{0,1}, \quad (3.10)$$

where

$$\Omega_{0,0} = -2 \int \frac{du}{2\pi} s^{(0)}(u) \frac{\rho^{(0)}(u)}{1 + \eta(u)}$$

and

$$\Gamma_{0,1} = 2 \int \frac{du}{2\pi} \left( \tilde{s}^{(1)}(u) \frac{\rho^{(0)}(u)}{1 + \eta(u)} + s^{(1)}(u) \frac{\sigma^{(0)}(u)}{1 + \eta(u)} \right).$$

### 3.2 Multiple strings

It is straightforward to extend the previous calculation to states with an arbitrary string content. Instead of repeating all the steps we merely present the results.

The mean value  $\langle \sigma_1^z \sigma_2^z \rangle_\Psi$  can be expressed by the same formula as in the 1-string case:

$$\langle \sigma_1^z \sigma_2^z \rangle_\Psi = 1 - \coth(\eta) \Omega_{0,0} + \Gamma_{0,1}. \quad (3.11)$$

However, in the general case all strings contribute and we have

$$\begin{aligned} \Omega_{0,0} &= -2s^{(0)} \cdot \frac{\rho^{(0)}}{1+\eta} \\ \Gamma_{0,1} &= 2 \left( \tilde{s}^{(1)} \cdot \frac{\rho^{(0)}}{1+\eta} + s^{(1)} \cdot \frac{\sigma^{(0)}}{1+\eta} \right). \end{aligned} \quad (3.12)$$

Here  $\rho^{(0)}$  are the total root densities which are solutions to (2.13) and  $\sigma^{(0)}$  is an auxiliary function satisfying

$$\sigma^{(0)} = \tilde{s}^{(0)} + \tilde{\varphi} \star \frac{\rho^{(0)}}{1+\eta} - \varphi \star \frac{\sigma^{(0)}}{1+\eta}. \quad (3.13)$$

In the formulas above we applied the notations introduced at the end of Section 2. The sources and kernels follow from the appropriate derivatives of the string propagators and string-string scattering phases. The one-particle functions are

$$\begin{aligned} s_k^{(0)}(u) &= (-i) [\cot(u + ik\eta/2) - \cot(u - ik\eta/2)] \\ s_k^{(1)}(u) &= i \left[ \frac{1}{\sin^2(u + ik\eta/2)} - \frac{1}{\sin^2(u - ik\eta/2)} \right] \\ \tilde{s}_k^{(0)}(u) &= \frac{k}{2} [\cot(u + ik\eta/2) + \cot(u - ik\eta/2)] \\ \tilde{s}_k^{(1)}(u) &= -\frac{k}{2} \left[ \frac{1}{\sin^2(u + ik\eta/2)} + \frac{1}{\sin^2(u - ik\eta/2)} \right]. \end{aligned} \quad (3.14)$$

The kernels  $\varphi_{nm}$  are given by (2.7), whereas  $\tilde{\varphi}_{nm}$  reads

$$\tilde{\varphi}_{nm} = \begin{cases} -(\tilde{s}_{|n-m|}^{(0)} + 2\tilde{s}_{|n-m|+2}^{(0)} + 2\tilde{s}_{|n-m|+4}^{(0)} + \cdots + 2\tilde{s}_{n+m-2}^{(0)} + \tilde{s}_{n+m}^{(0)}) & \text{if } m \neq n \\ -(2\tilde{s}_2^{(0)} + 2\tilde{s}_4^{(0)} + \cdots + 2\tilde{s}_{2n-2}^{(0)} + \tilde{s}_{2n}^{(0)}) & \text{if } m = n. \end{cases}$$

Equations (3.11)-(3.12) are a central result of this work. They are valid for arbitrary states with a smooth distribution of string centers given that the string hypothesis holds.

For the sake of completeness we note that the x-x correlator can be expressed using the relation  $\langle H \rangle / L = -\sinh(\eta) \Omega_{0,0}$  as

$$\langle \sigma_1^x \sigma_2^x \rangle_\Psi = \frac{1}{2 \sinh \eta} \Omega_{0,0} - \frac{\cosh \eta}{2} \Gamma_{0,1}.$$

## 4 The finite temperature case

In this section we consider finite temperature mean values of local correlators. They are defined as

$$\langle \mathcal{O} \rangle_T = \lim_{L \rightarrow \infty} \frac{\text{Tr } e^{-\beta H} \mathcal{O}}{Z(L)}, \quad Z(L) = \text{Tr } e^{-\beta H} = e^{-L\beta f(\beta)},$$

where  $\beta$  is the inverse temperature and  $f(\beta)$  is the free energy density.

Traditionally there are two different methods in the Bethe Ansatz literature to treat the finite temperature problem: the Quantum Transfer Matrix (QTM) method [21, 10] and the Thermodynamic Bethe Ansatz (TBA) [19]. Whereas they give the same result for the free energy density [22], only the QTM was known to provide the correlators as well. On the other hand, the TBA yields the finite temperature root distributions, which can be used as an input to our equations (3.11)-(3.12). This way we obtain an independent formula for  $\langle \sigma_1^z \sigma_2^z \rangle_T$  which can be compared to the known result of the QTM method.

In the following we collect the relevant results of the two approaches and we compare the predictions for the nearest neighbour correlator.

## 4.1 Short distance correlators in the QTM approach

In the QTM approach the central object is the auxiliary function  $\mathbf{a}(\lambda)$  which is a complex valued function over the complex plain and it is the solution of the integral equation

$$\log \mathbf{a}(\lambda) = 2\beta h - 2 \sinh(\eta) \beta q_+^{(0)}(\lambda) - \int_C \frac{d\omega}{2\pi i} K(\lambda - \omega) \log(1 + \mathbf{a}(\omega)). \quad (4.1)$$

Here  $\beta = 1/T$  is the inverse temperature,

$$K(u) = \frac{\sinh 2\eta}{\sinh(u + \eta) \sinh(u - \eta)},$$

and

$$q_+^{(0)}(\lambda) = \frac{\cosh(\lambda)}{\sinh(\lambda)} - \frac{\cosh(\lambda + \eta)}{\sinh(\lambda + \eta)}.$$

The free energy is computed as

$$f = h - T \int_C \frac{d\omega}{2\pi i} q_+^{(0)}(\omega) \log(1 + \mathbf{a}(\omega)).$$

The complex integrals run over a contour  $C$  which depends on the anisotropy  $\Delta$ . For  $\Delta > 1$  it can be chosen as the union of two straight line segments:

$$C = [i\pi/2 - \alpha, -i\pi/2 - \alpha] \cup [-i\pi/2 + \alpha, i\pi/2 + \alpha],$$

where  $\alpha < \eta/2$  is an arbitrary parameter which has to be chosen large enough so that the contour encircles all zeroes of the function  $1 + \mathbf{a}(\omega)$  in the domain  $|\text{Im}(\omega)| \leq \pi/2$ ,  $|\text{Re}(\omega)| \leq \eta/2$ .

Multiple integral formulas for the finite temperature correlation functions were first derived in [3]. Later it was shown in [11] that the multiple integrals can be factorized, i.e. they can be expressed as sums of products of simple integrals. The paper [23] also presents numerical data for the short range correlators for the  $\Delta > 1$  regime.

In the following we present the formulas extracted from [11] which are necessary for the practical computations. Let us define the auxiliary functions  $G_a(\lambda)$  and  $\tilde{G}_a(\lambda)$ ,  $a = 0 \dots \infty$ , which are solutions to the linear integral equations

$$G_j(\lambda) = q_-^{(a)}(\lambda) + \int_C \frac{d\omega}{2\pi i} K(\lambda - \omega) \frac{G_a(\omega)}{1 + \mathbf{a}(\omega)} \quad (4.2)$$

and

$$\tilde{G}_a(\lambda, \mu) = \tilde{q}_-^{(a)} + \int_C \frac{d\omega}{2\pi i} \frac{G_a(\omega)}{1 + \mathbf{a}(\omega)} \tilde{K}(\lambda - \omega) + \int_C \frac{d\omega}{2\pi i} \frac{\tilde{G}_a(\omega)}{1 + \mathbf{a}(\omega)} K(\lambda - \omega),$$

where

$$\begin{aligned} \tilde{q}_-^{(a)} &= \left( -\frac{\partial}{\partial \lambda} \right)^a \coth(\lambda - \eta) \\ q_-^{(a)} &= \left( -\frac{\partial}{\partial \lambda} \right)^a (\coth(\lambda - \eta) - \coth(\lambda)) \end{aligned}$$



and

$$\tilde{K}(u) = \frac{\sinh(2u)}{\sinh(u+\eta)\sinh(u-\eta)}.$$

Let the numbers  $\Psi_{a,b}$  and  $P_{a,b}$  with  $a, b = 0 \dots \infty$  be given by

$$\begin{aligned}\Psi_{a,b} &= \int_C \frac{d\omega}{\pi i} q_-^{(b)}(\omega) \frac{G_a(\omega)}{1 + \mathfrak{a}(\omega)} \\ P_{a,b} &= \int_C \frac{d\omega}{\pi i} \left[ q_-^{(b)}(\omega) \frac{\tilde{G}_a(\omega)}{1 + \mathfrak{a}(\omega)} + \tilde{q}_-^{(b)}(\omega) \frac{G_a(\omega)}{1 + \mathfrak{a}(\omega)} \right].\end{aligned}\tag{4.3}$$

These objects are the building blocks for the local correlations. As a final step we define

$$\begin{aligned}\omega_{a,b} &= -\Psi_{a,b} - (-1)^b \frac{1}{2} \left( \frac{\partial}{\partial u} \right)^{a+b} K(u) \Big|_{u=0} \\ W_{a,b} &= -P_{a,b} + (-1)^b \frac{1}{2} \left( \frac{\partial}{\partial u} \right)^{a+b} \tilde{K}(u) \Big|_{u=0}.\end{aligned}\tag{4.4}$$

They possess the symmetry properties

$$\omega_{a,b} = \omega_{b,a} \quad W_{a,b} = -W_{b,a}.$$

All short distance correlators can be expressed as a combination of the numbers  $\omega_{a,b}$  and  $W_{a,b}$ . The formulas can be found in the papers [11, 23] <sup>1</sup>. Here we present four examples:

$$\begin{aligned}\langle \sigma_1^z \sigma_2^z \rangle_T &= \coth(\eta) \omega_{0,0} + W_{1,0} \\ \langle \sigma_1^x \sigma_2^x \rangle_T &= -\frac{\omega_{0,0}}{2 \sinh(\eta)} - \frac{\cosh(\eta)}{2} W_{1,0} \\ \langle \sigma_1^z \sigma_3^z \rangle_T &= 2 \coth(2\eta) \omega_{0,0} + W_{1,0} + \tanh(\eta) \frac{\omega_{2,0} - 2\omega_{1,1}}{4} - \frac{\sinh^2(\eta)}{4} W_{2,1} \\ \langle \sigma_1^x \sigma_3^x \rangle_T &= -\frac{1}{\sinh(2\eta)} \omega_{0,0} - \frac{\cosh(2\eta)}{2} W_{1,0} - \tanh(\eta) \cosh(2\eta) \frac{\omega_{2,0} - 2\omega_{1,1}}{8} + \\ &\quad + \sinh^2(\eta) \frac{W_{2,1}}{8}.\end{aligned}\tag{4.5}$$

Using (4.4) the nearest neighbour  $z - z$  correlator is expressed as

$$\langle \sigma_1^z \sigma_2^z \rangle_T = 1 - \coth(\eta) \Psi_{0,0} + P_{0,1},\tag{4.6}$$

where we used  $P_{0,1} = -P_{1,0}$ .

## 4.2 The nearest neighbour correlator from TBA

The Thermodynamic Bethe Ansatz was devised to determine the free energy density by finding a saddle point distribution to the free energy functional [24, 19]. In the case of the XXZ spin chain with  $\Delta > 1$  the TBA yields the following set of nonlinear integral equations for the functions  $\eta_k(u)$  defined in (2.8):

$$\log \eta_k(u) = -2k\beta h + 2 \sinh(\eta) \beta s_k^{(0)}(u) + \sum_{j=1}^{\infty} \int_{-\pi/2}^{\pi/2} \frac{d\omega}{2\pi} \varphi_{kj}(u - \omega) \log(1 + 1/\eta_j(\omega)).\tag{4.7}$$

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<sup>1</sup>Our notation differs slightly from [11, 23]: Our  $\omega$  and  $W$  correspond to  $\omega$  and  $\omega'/\eta$  of [11, 23], respectively, and we denote the number of derivatives with respect to the variables  $x$  and  $y$  by  $a$  and  $b$ . For example  $W_{1,2} = \omega'_{xyy}/\eta$ .

The free energy density can then be expressed as

$$f = h + T \sum_{k=1}^{\infty} \int_{-\pi/2}^{\pi/2} \frac{du}{2\pi} s_k^{(0)}(u) \log(1 + 1/\eta_j(\omega)).$$

In (4.7) all  $\eta_k$  are coupled through the kernels  $\varphi_{kj}$ . A simpler form of the TBA equations can be derived where only neighbouring equations are coupled [19]; however, it will not be used here.

If the  $\eta_k$  are found from (4.7) then formulas (3.11)-(3.13) can be used to find the densities, the auxiliary functions  $\sigma_k^{(0)}$  and finally the finite temperature mean value  $\langle \sigma_1^z \sigma_2^z \rangle_T$ .

In order to check our results we numerically computed  $\langle \sigma_1^z \sigma_2^z \rangle_T$  for different values of  $\Delta$ ,  $\beta$  and  $h$  from both the TBA and the QTM formulas. We found convincing numerical evidence that the two approaches give the same results; examples of the numerical data are presented in the Appendix.

## 5 Conjectures for the short range correlators

It is hard to miss the conspicuous similarities between the QTM and Bethe Ansatz (BA) formulas for  $\langle \sigma_1^z \sigma_2^z \rangle_T$ : there is a formal one-to-one correspondence at each step of the calculation, even though on the BA side we have an infinite number of equations, whereas on the QTM side there are only two. It is easy to see that the building blocks of the formulas coincide:

$$\Omega_{0,0} = \Psi_{0,0} \quad \Gamma_{0,1} = P_{0,1}. \quad (5.1)$$

The first equation follows from the fact that both  $\Omega_{0,0}$  and  $\Psi_{0,0}$  are proportional to the mean value of the Hamiltonian, whereas the second follows from the equality of the two formulas for the correlator given that the first relation is already established.

Based on these observations we generalize the formulas of Section 2 as follows. Let  $\rho^{(a)}$  and  $\sigma^{(a)}$  for general  $a \geq 0$  be given as the unique solution to the linear equations

$$\rho^{(a)} = -s^{(a)} - \varphi \star \frac{\rho^{(a)}}{1 + \eta} \quad (5.2)$$

$$\sigma^{(a)} = \tilde{s}^{(a)} + \tilde{\varphi} \star \frac{\rho^{(a)}}{1 + \eta} - \varphi \star \frac{\sigma^{(a)}}{1 + \eta}. \quad (5.3)$$

Here

$$s^{(a)}(u) = \left( \frac{\partial}{\partial u} \right)^a s^{(0)}(u) \quad \tilde{s}^{(a)}(u) = \left( \frac{\partial}{\partial u} \right)^a \tilde{s}^{(0)}(u).$$

We define the numbers  $\Omega_{a,b}$  and  $\Gamma_{a,b}$  as

$$\Omega_{a,b} = -2s^{(b)} \cdot \frac{\rho^{(a)}}{1 + \eta} \quad (5.4)$$

and

$$\Gamma_{a,b} = 2 \left( \tilde{s}^{(b)} \cdot \frac{\rho^{(a)}}{1 + \eta} + s^{(b)} \cdot \frac{\sigma^{(a)}}{1 + \eta} \right). \quad (5.5)$$

We propose the following two conjectures.

**Conjecture 1.** *In the finite temperature situation the building blocks of the QTM formulas for correlators can be computed from the string densities only. That is,*

$$\Omega_{a,b} = (-1)^{(a+b)/2} \Psi_{a,b} \quad \text{and} \quad \Gamma_{a,b} = (-1)^{(a+b-1)/2} P_{a,b}, \quad a, b = 0 \dots \infty, \quad (5.6)$$

given that  $\Omega_{a,b}$  and  $\Gamma_{a,b}$  are calculated from (5.2)-(5.5) with  $\eta_k(u)$  being the solution of the TBA equation (4.7) and  $\Psi_{a,b}$  and  $P_{a,b}$  are calculated from (4.3) with  $\mathfrak{a}(u)$  being the solution of the NLIE (4.1) with the same inverse temperature and magnetic field.

The sign factors in (5.6) can be understood by noticing that the QTM and TBA rapidity parameters are related by a rotation of  $90^\circ$  in the complex plane. This results in factors of  $i$  whenever the formulas for the sources are differentiated. The overall sign of  $\Omega$  and  $\Gamma$  is fixed by the identities (5.1) which follow from their definition and the Hellmann–Feynman theorem.

We numerically checked Conjecture 1 and convinced ourselves that it holds for arbitrary anisotropy, temperatures and magnetic fields; examples of the correlators computed using Conjecture 1 are presented in the Appendix. It follows that the finite temperature correlators can be obtained from the TBA string densities only. While this procedure is numerically more costly than the pure QTM calculation, our second conjecture states that the validity of the Bethe Ansatz formulas might be more general and not restricted to the finite temperature situation.

**Conjecture 2.** *Short distance correlators in any Bethe state with smooth distribution of string centers can be computed via the following procedure:*

1. Compute the auxiliary functions  $\rho^{(a)}$  and  $\sigma^{(a)}$  from (5.2) and (5.3).
2. Compute  $\Omega_{a,b}$  and  $\Gamma_{a,b}$  from (5.4) and (5.5).
3. Use the relations

$$\begin{aligned}\omega_{a,b} &= -(-1)^{(a+b)/2}\Omega_{a,b} - (-1)^b \frac{1}{2} \left( \frac{\partial}{\partial u} \right)^{a+b} K(u) \Big|_{u=0} \\ W_{a,b} &= -(-1)^{(a+b-1)/2}\Gamma_{a,b} + (-1)^b \frac{1}{2} \left( \frac{\partial}{\partial u} \right)^{a+b} \tilde{K}(u) \Big|_{u=0}\end{aligned}\tag{5.7}$$

to obtain  $\omega_{a,b}$  and  $W_{a,b}$ .

4. Substitute  $\omega_{a,b}$  and  $W_{a,b}$  into the already available factorized formulas of the QTM literature. Examples for two-site and three-site correlators are presented in (4.5).

We have shown that Conjecture 2 is true for the nearest neighbour correlator with arbitrary string distributions, and numerical evidence supports its validity for all local correlators in the finite temperature case. It is an open question whether it is true in full generality.

## 6 Discussion and Outlook

We derived an analytical formula for the simplest non-trivial correlator  $\langle \sigma_1^z \sigma_2^z \rangle_\Psi$  which is valid for Bethe states with arbitrary string distributions. Our result could be used in quantum quench problems to give prediction for the long-time limit of this particular observable, if the root densities can be determined from the quench action [5, 15, 16, 17].

Based on very close similarities with known formulas from the QTM approach we conjectured a generalization to other short distance correlators. If Conjecture 2 is found to be true, it would give a new interpretation to the factorized formulas of [11]. And even if it is not true, it still needs to be understood why it works in the finite temperature case (see Conjecture 1 and the numerical data in the Appendix).

We think it is worthwhile to recall a situation which seems to be analogous to the present one. In [25] an infinite integral series was derived for the  $K$ -body local correlators of the 1D Bose gas; the idea for this series originated from the theory of integrable QFT's where it is called the LeClair–Mussardo (LM) series. The result of [25] holds for an arbitrary distribution of Bethe roots. In [26] the LM series was summed up into simple formulas in the cases  $K = 2, 3$ . Later a different multiple integral formula was found in [27] which was factorized for  $K \leq 4$ , reproducing the earlier results of [26]. It is very important that all of these calculations are completely general in the sense that they do not rely on any assumption of an underlying thermal ensemble. The only input to the factorized formulas is the filling fraction  $\rho_r(\lambda)/\rho(\lambda)$ , which is treated as an arbitrary function.

We believe that a LeClair–Mussardo series could be established also for the local operators of the XXZ chain using the methods of [25]. If such a series exists, then its application for ground state or finite temperature correlations would be far less effective than any of the existing methods, but it would be valid for arbitrary string distributions. Moreover, the conjectured results of the present work could follow from a summation of the LM series. We leave these questions to further research.

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## Notes added:

The conjectured formulas of this work were used in the paper [17] to give predictions for the long-time limit of local correlations following a quantum quench. In all cases perfect agreement was found with the results of real-time numerical simulations, and this provides strong evidence for the validity of Conjecture 2.

Our results for the nearest neighbour z-z correlator presented in Section 3 were obtained independently in the paper [16], which was submitted as an e-print to the arXiv on the same day as the present work.

## A Numerical checks

We numerically checked Conjecture 2 in the finite temperature situation by computing both the QTM and TBA formulas for the quantities  $\omega_{a,b}$  and  $W_{a,b}$  and substituting them into the factorized formulas for the short distance two-point functions. We truncated the infinite set of TBA equations and observed that the truncation number needed to obtain good agreement with the QTM results strongly depends on the temperature and the magnetic field. For large negative magnetic fields and small temperatures the higher strings are suppressed; we observed that in many cases perfect numerical agreement can be found already with  $\leq 10$  equations. On the other hand, if at a finite (non-zero) temperature the magnetic field is zero or very small then the contributions of the higher strings can be considerable and a large number of equations is required. In such cases we found that instead of equations (5.2)-(5.3) it is more efficient to use the decoupled form which can be written as follows.

Consider an equation of the type

$$f_k(u) = g_k(u) - \sum_{l=1}^{\infty} \int_{-\pi/2}^{\pi/2} \frac{d\omega}{2\pi} \varphi_{kl}(u - \omega) \frac{f_k(\omega)}{1 + \eta_k(\omega)}. \quad (\text{A.1})$$

Applying the well-known steps to decouple the convolution terms results in [19]

$$\begin{aligned} f_k(u) = g_k(u) - \int_{-\pi/2}^{\pi/2} \frac{d\omega}{2\pi} s(u - \omega) (g_{k-1}(u) + g_{k+1}(u)) + \\ + \int_{-\pi/2}^{\pi/2} \frac{d\omega}{2\pi} s(u - \omega) \left( \frac{\eta_{k+1}(\omega) f_{k+1}(\omega)}{1 + \eta_{k+1}(\omega)} + \frac{\eta_{k-1}(\omega) f_{k-1}(\omega)}{1 + \eta_{k-1}(\omega)} \right), \end{aligned} \quad (\text{A.2})$$

where

$$s(x) = 1 + 2 \sum_{n=1}^{\infty} \frac{\cos(2nx)}{\cosh(\eta n)}.$$

	$N = 2$	$N = 4$	$N = 10$	QTM
$\langle \sigma_1^z \sigma_2^z \rangle_T$	$-1.7663637 \cdot 10^{-1}$	$-1.7678391 \cdot 10^{-1}$	$-1.7678511 \cdot 10^{-1}$	$-1.7678511 \cdot 10^{-1}$
$\langle \sigma_1^x \sigma_4^x \rangle_T$	$-5.7948070 \cdot 10^{-3}$	$-5.5484712 \cdot 10^{-3}$	$-5.5455688 \cdot 10^{-3}$	$-5.5455688 \cdot 10^{-3}$

(a)  $\Delta = 3, \beta = 0.2, h = -1$

	$N = 10$	$N = 20$	$N = 30$	QTM
$\langle \sigma_1^z \sigma_2^z \rangle_T$	$-4.7190677 \cdot 10^{-1}$	$-4.7183624 \cdot 10^{-1}$	$-4.7183623 \cdot 10^{-1}$	$-4.7183623 \cdot 10^{-1}$
$\langle \sigma_1^x \sigma_4^x \rangle_T$	$-7.1256853 \cdot 10^{-3}$	$-6.9050701 \cdot 10^{-3}$	$-6.9050442 \cdot 10^{-3}$	$-6.9050445 \cdot 10^{-3}$

(b)  $\Delta = 3, \beta = 0.2, h = -0.4$

	$N = 10$	$N = 20$	$N = 40$	QTM
$\langle \sigma_1^z \sigma_2^z \rangle_T$	$-5.2791241 \cdot 10^{-1}$	$-5.2480411 \cdot 10^{-1}$	$-5.2459375 \cdot 10^{-1}$	$-5.24591662 \cdot 10^{-1}$
$\langle \sigma_1^x \sigma_4^x \rangle_T$	$-1.227053385 \cdot 10^{-2}$	$-7.4127763 \cdot 10^{-3}$	$-7.1443727 \cdot 10^{-3}$	$-7.14182791 \cdot 10^{-3}$

(c)  $\Delta = 3, \beta = 0.2, h = -0.1$

	$N = 10$	$N = 20$	$N = 40$	QTM
$\langle \sigma_1^z \sigma_2^z \rangle_T$	$-6.6205394 \cdot 10^{-1}$	$-6.5927266 \cdot 10^{-1}$	$-6.5869615 \cdot 10^{-1}$	$-6.5852520 \cdot 10^{-1}$
$\langle \sigma_1^x \sigma_4^x \rangle_T$	$-5.0765570 \cdot 10^{-3}$	$-4.7597568 \cdot 10^{-3}$	$-4.7526870 \cdot 10^{-3}$	$-4.74751256 \cdot 10^{-3}$

(d)  $\Delta = 2, \beta = 0.5, h = 0$

Table 1: Examples of the numerical results for the finite temperature local correlators. The first three columns present the calculations with the truncated TBA system with  $N$  equations, whereas the last column is the numerically exact result of the QTM method.

This means a drastic simplification in the equation of  $\rho^{(a)}$  because all source terms disappear except for  $k = 1$ :

$$\begin{aligned} \rho_k^{(a)}(u) = & \delta_{k,1} \left( \frac{\partial}{\partial u} \right)^a s(u) + \\ & + \int_{-\pi/2}^{\pi/2} \frac{d\omega}{2\pi} s(u - \omega) \left( \frac{\eta_{k+1}(\omega) \rho_{k+1}^{(a)}(\omega)}{1 + \eta_{k+1}(\omega)} + \frac{\eta_{k-1}(\omega) \rho_{k-1}^{(a)}(\omega)}{1 + \eta_{k-1}(\omega)} \right). \end{aligned} \quad (\text{A.3})$$

There is a similar formula for  $\sigma^{(a)}$  which will be presented elsewhere.

Examples of our numerical data are shown in Table 1. We computed the local correlators  $\langle \sigma_1^a \sigma_{1+j}^a \rangle_T$  with  $a = z, x$  and  $j = 1, 2, 3$  for various values of the triplets  $(\Delta, \beta, h)$ . For the sake of brevity here we only present results for  $\langle \sigma_1^z \sigma_2^z \rangle_T$  and  $\langle \sigma_1^x \sigma_4^x \rangle_T$  in 4 different situations.

In the first case we chose a relatively large magnetic field. Here  $N = 10$  equations sufficed to obtain the correct result up to 8 digits; we used the original linear equations. Note that even though the  $N = 10$  result is already accurate to the digits given, the  $N = 2$  and  $N = 4$  truncations still show small differences.

In the other three cases the magnetic field was chosen to be smaller or zero. Accordingly a larger number of equations was required; in these cases we used the decoupled form of the linear integral equations. The TBA data always seems to converge to the QTM result, but for very small or zero magnetic fields we found a relative error of the order  $10^{-3}$  even at  $N = 40$ , where our current computer programs are already slow. We conclude that in these situations the strings that are longer than 40 still contribute considerably and our programs need to be improved to be able to handle these cases as well.

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